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A comparison of two equations of state

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Abstract: The forms of two astrophysically applicable equations of state (EOS) are compared: the EOS proposed within the semiclassical theory of dense matter developed by P.Savic and R.Kasanin, and the universal equation of state introduced by Vinet et.al. Some similarities between them are discussed, and possibilities of astrophysical tests are pointed out.

Introduction

In physics, astrophysics and related sciences, the term "equation of state" (EOS) denotes any kind of relationship between the parameters describing the state of the system. In the case of a thermomechanical system, the general form of the EOS is $f(p, V, T) = 0$. The symbols p , V and T denote, respectively, the pressure, volume and temperature of the system under consideration. Establishing the EOS of any given system (or class of systems) is a complicated problem in experimental and theoretical physics. Results of these studies are of paramount importance in astrophysics, in problems ranging from the analysis of the propagation of seismic waves through the Earth, through studies of planetary and stellar internal structure, to the evolution of the early Universe.

The aim of this contribution is to compare two EOS of solids under high pressure. One of them has been proposed (although not in fully explicit form) in the so-called SK theory of the behaviour of materials under high pressure, developed by P.Savic and R.Kasanin (Savic and Kasanin, 1962/65) and later authors.

The other equation (called the universal EOS) has been proposed relatively recently (Vinet et al.,1989 and earlier work). The interest in comparing these two EOS stems from the fact that they are both applicable to planetologically important materials. It was very recently shown that the EOS of Vinet et al is applicable to high compression (Cohen, Gulseren and Hemley,1999).

Calculations

This section contains a brief derivation of the EOS within the SK theory. Some details of this calculation were published previously (Celebonovic,1996), but, in order to correct some misprints the calculation is repeated here. In the calculation, the subscript i denotes the ordinal number of the phase of the substance.

It can be shown within the SK theory that the function $\partial P/\partial \rho$ has the following form:

$$\frac{\partial P}{\partial \rho} = \frac{N_A e^2}{9A} Q_i \quad (1)$$

where

$$Q_i = \frac{4}{a_i} f_i(a_i) - f'_i(a_i) \quad (2)$$

and N_A, e, A denote, respectively, Avogadro's number, the electron charge and the mean atomic mass of the specimen. The function $f_i(a_i)$ is given by

$$f_i(a_i) = C_i + B_i \exp[\gamma_i z_i] \quad (3)$$

in which

$$a_i = \left(\frac{A}{8N_A \rho_i} \right)^{1/3} \quad (4)$$

and

$$z_i = (1 - a_i^*/a_i)/(1 - \alpha_i^{-1/3}) \quad (5)$$

Inserting eq.(3) into eq.(2) it follows that

$$Q_i = \frac{4}{a_i} (C_i + B \exp[\gamma_i z_i] - \gamma_i z_i \frac{\partial z_i}{\partial a_i} \exp[\gamma_i z_i]) \quad (6)$$

where α, γ, B, C are constants within a given phase i , whose numerical values are known within the SK theory. Expressing $\frac{\partial z}{\partial a}$ as $\frac{\partial z}{\partial \rho} \frac{\partial \rho}{\partial a}$, after some algebra one arrives at the following :

$$Q_i = 8 \left(\frac{N_A \rho}{A} \right)^{1/3} \left[C_i + B_i \left[1 - W_i \rho_i \left(\frac{\rho_i}{\rho_i^*} \right)^{1/3} \right] \right] \exp 4W \left[1 - \left(\frac{\rho_i}{\rho_i^*} \right)^{1/3} \right] \quad (7)$$

and

$$W_i = \frac{\gamma_i}{1 - \left(\frac{\rho_i}{\rho_i^*} \right)^{1/3}} \quad (8)$$

The isothermal bulk-modulus, defined by $B = \rho \partial P / \partial \rho$, is obviously density dependent. Inserting eq.(7) into eq.(1) and integrating withn a given phase i of the material under pressure, one gets the explicite form of the EOS in ths SK theory. The first few terms of this equation are:

$$P(\rho_i) = \frac{2e^2}{3} \left(\frac{N_A}{A} \right)^{1/3} \rho_i^{4/3} \left[C_i \frac{N_A}{A} + B_i \rho_i \exp \left[4W_i \left(1 - (\rho_i / \rho_i^*)^{1/3} \right) + .. \right] \right] \quad (9)$$

Note that the zero of the pressure scale is placed at the value of the pressure corresponding to the lower limit of the density of a the phase. The symbol ρ_i^* denotes the maximal density in the phase.

The EOS proposed by Vinet et al. (1989, and earlier work) has the following form

$$P(\rho) = 3B \frac{1-x}{x^2} \exp \left[\frac{3}{2} (B' - 1)(1-x) \right] \quad (10)$$

where $x = (V/V_0)^{1/3} = (\rho_0/\rho)^{1/3}$ and the next section is devoted to a brief comparison of eqs.(9) and (10) .

The comparison and conclusions

Briefly stated, there are similarities in the method by which eqs.(9) and (10) were derived. The EOS of SK is a result of a set of experimentally verified postulates and a selection rule. It presupposes a pure Coulomb interatomic interaction potential, but with a "hidden" hard core (Celebonovic, 1999b and earlier work). On the other hand, the Vinet et al. theory includes additional terms apart from the pure Coulomb in the interaction potential, but presupposes a form of the scaling of energy. The scaling length in their theory depends on the Wigner-Seitz radius at normal pressure, which has been shown to enter in the definition of the interatomic distance in SK. The bulk modulus in SK is a function of the density, which can be calculated in the theory. In eq.(10) it is a constant, whose value can be obtained by fitting eq.(10) to experimental data.

A short general conclusion can be that the EOS of SK and Vinet et al. show certain similarities, but that eq.(10) is physically more realistic because it takes into account more terms in the interaction potential. The next step could be the application of both of these EOS to a cold astrophysical object, such as a planet, obtaining a model and comparing it to the observable parameters of the object.

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